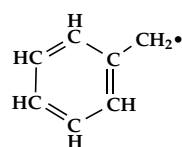


THERMAL DECOMPOSITION OF C₇H₇ RADICALS; BENZYL, TROPYL, AND NORBORNADIENYL

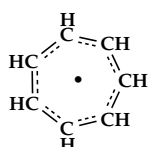
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Benzyl radical (C₆H₅CH₂) and two other C₇H₇ radicals are commonly encountered in the combustion of substituted aromatic compounds found in biofuels and gasoline. High temperature pyrolysis of benzyl radical requires isomerization to other C₇H₇ radicals that may include cycloheptatrienyl (troyl) radical (*cyc*-C₇H₇) and norbornadienyl radical. The thermal decomposition of all three radicals has now been investigated using a micro-reactor that heats dilute gas-phase samples up to 1600 K and has a residence time of about 100 μ -sec. The pyrolysis products exit the reactor into a supersonic expansion and are detected using synchrotron-based photoionization mass spectrometry and matrix-isolation IR spectroscopy. The products of the pyrolysis of benzyl radical (C₆H₅CH₂) along with three isotopomers (C₆H₅¹³CH₂, C₆D₅CH₂, and C₆H₅CD₂) were detected and identified^a. The distribution of ¹³C atoms and D atoms indicate that multiple different decomposition pathways are active.

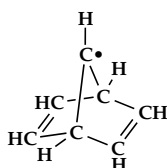
^aBuckingham, G. T., Ormond, T. K., Porterfield, J. P., Hemberger, P., Kostko, O., Ahmed, M., Robichaud, D. J., Nimlos, M. R., Daily, J. W., Ellison, G. B. 2015, *Journal of Chemical Physics* **142** 044307



benzyl radical
 \tilde{X}^2B_1



troyl radical
 \tilde{X}^2E_2''



norbornadienyl radical
 \tilde{X}^2B_1